# Lattice QCD for Nuclear Physics

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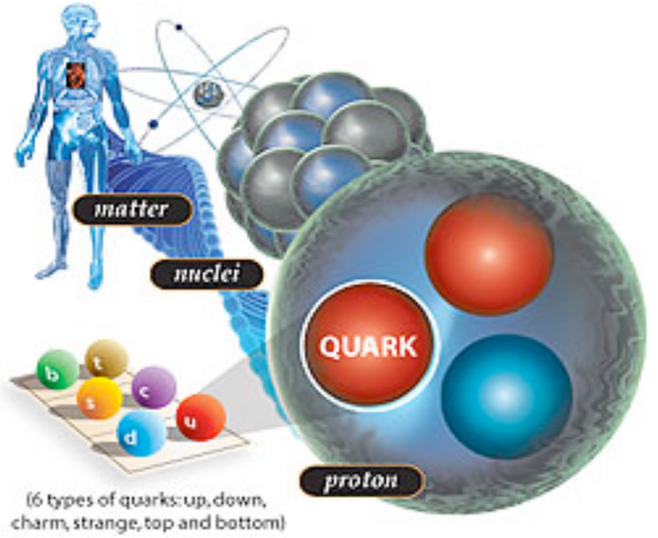
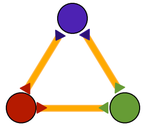
# Introduction

- It is believed that the fundamental building blocks of matter are ***quarks*** bound together by ***gluons***, via the ***strong nuclear force.***
- Quantum Chromodynamics (QCD) is the theory which describes the strong interactions
- Understanding how QCD makes up matter and how quarks and gluons behave is a subject of intense experimental scrutiny
  - only ~5% of the mass of a proton comes from mass of the quarks, rest comes from binding
  - gluon self-coupling and gluon excitations can create ***exotic forms of matter***

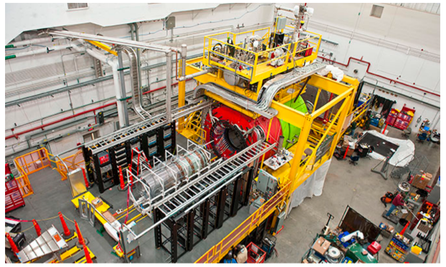



meson: 2 quarks



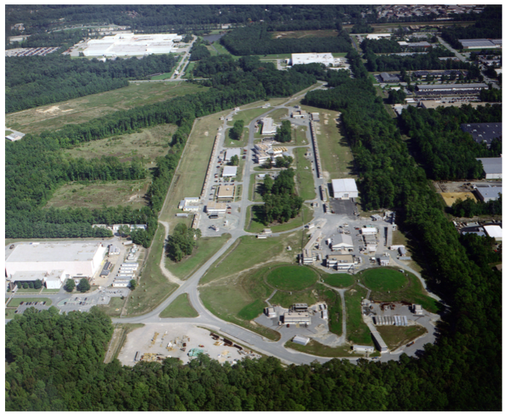
baryon: 3 quarks

glueball: 0 quarks only gluons



***GlueX in the new Hall-D of Jefferson Lab@12 GeV. Hunting for exotics!***

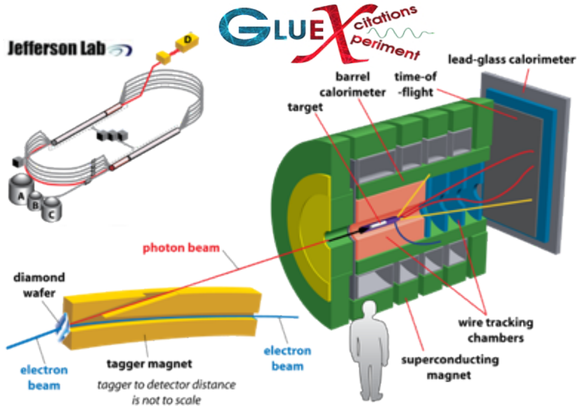
***Jefferson Lab***

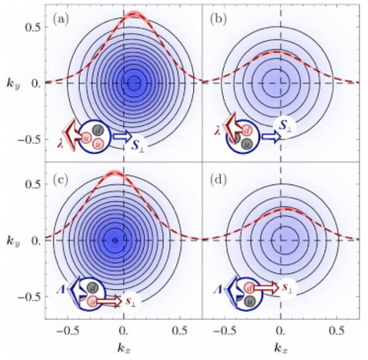


***Brookhaven National Lab***

# Important questions in Nuclear Physics

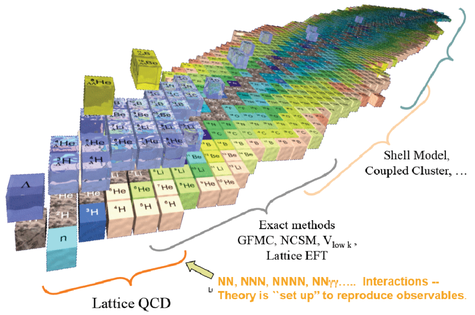
- What observable states does QCD allow?
  - what is the role of the gluons?
  - what about exotic matter?



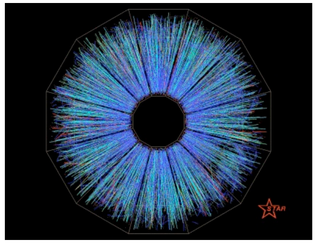
Hägler, Musch, Negele, Schäfer, EPL 88 61001

- How does QCD make protons, neutrons?
  - what are the distribution of quarks, gluons, etc in a proton or neutron ?




- QCD must predict properties of light nuclei
  - how to make helium, tritium etc

- How does QCD behave under extreme temperatures & pressures such as in supernovae or shortly after the Big-Bang.



# QCD: Path Integral Formulation

- Quarks and Gluons are ‘fields’ in space-time (Minkowski Space)
- QCD Is defined by the Action (S) over the fields
- Action enumerates potential interactions
  - quark-gluon, gluon-gluon etc.
- **Observables** can be computed through Path Integrals over the fields.
- Running Coupling (Asymptotic Freedom)
  - Large energies => Perturbation Theory
  - Low energy => Nonperturbative Method needed.

“Functional Integral” over all the possible states of the fields

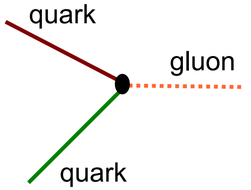
The “action” defining the theory

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}A \, \mathcal{D}\bar{\psi} \, \mathcal{D}\psi \, \mathcal{O} \, e^{-S(A,\bar{\psi},\psi)}$$

Expectation value of an observable (correlation function)

Value of observable on a concrete set of fields

$$S = \int dx \; dy \; \bar{\psi}(y) M(A; y, x) \psi(x)$$




$$-\int dx \; \frac{1}{4} G_a^{\mu\nu}(x) G^a_{\mu\nu}(x)$$

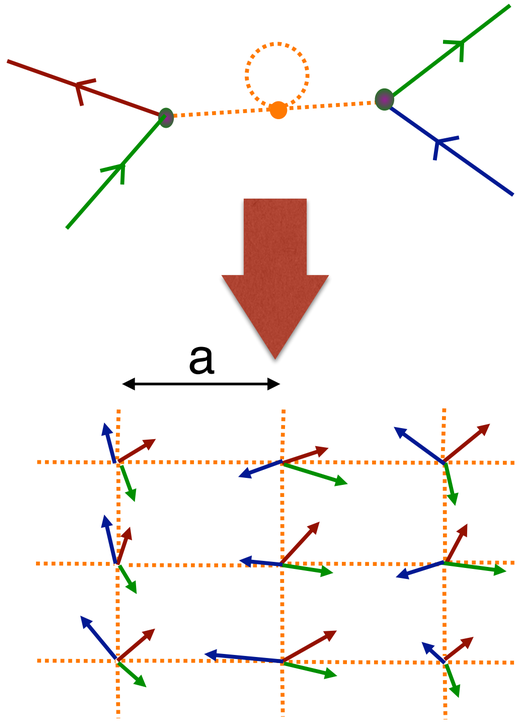
# Lattice QCD

- Replace “continuum” space time by 4D Lattice
  - 3D spatial box (finite volume)
  - Euclidean Time ( t => it ) ***$L_t$ is proportional to 1/Temperature***
- Discretize quark fields onto lattice sites
- Discretize gluon fields onto lattice links as SU(3) matrices

$$U_\mu(x) = \exp\left\{ ig \int_x^{x+\hat{\mu}} dx\ A_\mu(x) \right\} \approx \exp\{ig\ a\ A_\mu(x)\}$$

  - 3x3 matrices on links act as “parallel transporters” along links
- Finite differences for derivatives
- Functional integrals become ‘regular’ integrals
- QCD is continuum limit of LQCD (RG)
- LQCD is not a ``model”: Fully renormalizable QFT!!!

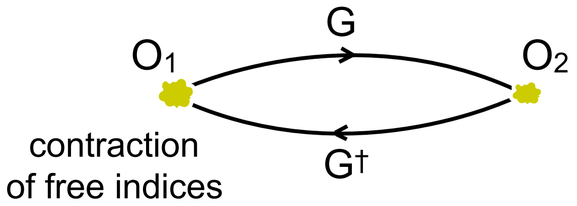
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}A\ \mathcal{D}\bar{\psi}\ \mathcal{D}\psi\ \mathcal{O}\ e^{-S(A,\bar{\psi},\psi)}$$




$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\text{all links}} dU \prod_{\text{all sites}} d[\bar{\psi},\psi]\ \mathcal{O}\ e^{-S(U,\bar{\psi},\psi)}$$

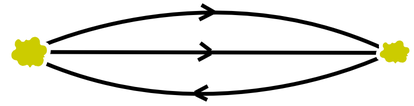
# What are our observables?

- Lattice QCD Observables are “correlation functions”
- E.g. For mesons (quark-antiquark pairings):




Meson: e.g. the π meson (a.k.a pion)

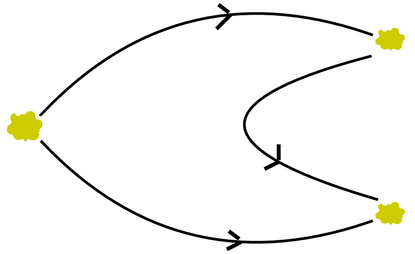
$$C(\vec{p},t) = \sum e^{i\vec{p}.\vec{x}}\ \mathrm{Tr}\ \{O_1\ G_1^\dagger\ O_2\ G_2\} = \sum A_i\ e^{-\sqrt{E_i^2+|\vec{p}|^2}t} \xrightarrow[t\to\infty]{} A_0\ e^{-\sqrt{m^2+|\vec{p}^2|}t}$$



Baryon: e.g. proton or neutron

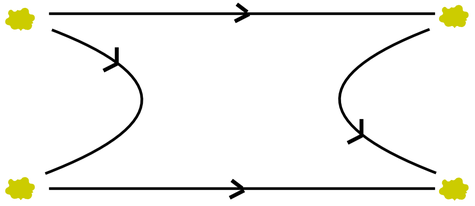
- G is the quark propagator defined as:

$$G(x,y) = M^{-1}_{x,y} S(x)$$



Meson to 2 meson decay: e.g. ρ → 2π

- M is the Fermion matrix
- Computing C(t) involves ***solving linear systems for G*** (Solvers) and ***contractions (few index)***



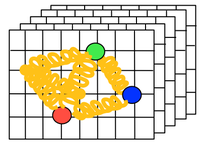
2 meson in to 2 meson out: e.g. 2π → 2π

# The name of the game:

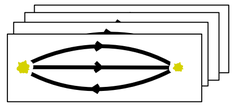
- ***Produce Ensembles of Configurations***
  - Several box-sizes for finite V behavior
    - E.g. Luscher formalism for phase shifts, resonances etc.
    - Several Temperatures (in Finite temperature calculations)
  - Several lattice spacings ‘a’ (to allow for continuum limit extraction)
  - As high statistics as possible (sample path integral well)
    - ***Want to minimize time for sample generation, minimize autocorrelation time (algorithms)***
- ***Evaluate Correlation Functions***
  - Need ***O(100,000)-O(1M)*** quark propagators per configuration (reduce signal to noise)
    - ***Want the fastest possible multi-RHS linear solvers***
  - Can have ***O(10,000)-O(100,000)*** quark line diagrams for some observables
    - ***Want to eliminate as many diagrams as possible using symmetry***
    - ***Want fast I/O for database accesses***
    - ***Want to maximize common by-product reuse***
    - ***Want automation & job orchestration: Workflows!!!!***
- ***Want to run on any hardware that falls into our lap:*** ***Performance portability Strategy***

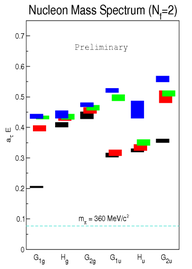
# Anatomy of an LQCD calculation


Gauge Configurations




Propagators, Correlation Functions






Gauge Generation: {U}

Measurement: O(U)

Fitting

Physics Result

- Gauge Generation: create snapshots of the LQCD Vacuum
  - sequential (Markov Chain) but has data parallelism from the lattice
  - strong scaling limited: needs leadership computing resources
- Measurement:
  - computes propagation of quarks on the gauge field snapshots
  - contracts propagators into correlation functions
  - throughput limited: very cost effective on clusters like at JLab or ensemble mode running at LCFs

*Titan Image Courtecy of OLCF*
*Edison Image Courtesy of NERSC*

# Importance Sampling

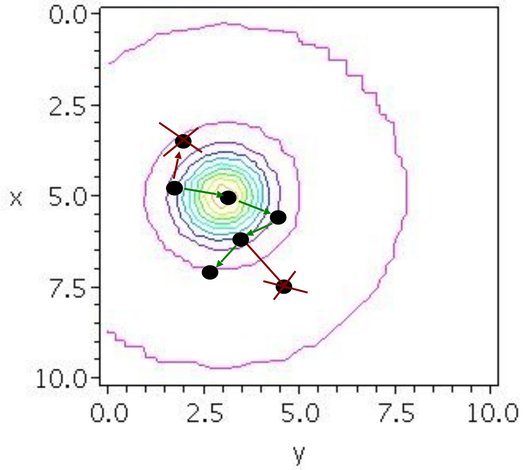
- Pick Configuration ‘U’ with probability P(U)
- Ensemble average then becomes a ‘regular average’

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\text{all links}} dU_i \; \mathcal{O} \; e^{-S(U)} \longrightarrow \bar{O} = \frac{1}{N} \sum_{\text{N}} \mathcal{O}(U) \qquad \sigma(\bar{\mathcal{O}}) \propto \frac{1}{\sqrt{N}}$$

- E.g.: Metropolis Algorithm
  - Start from some initial configuration U
  - Pick trial config U’ from U **reversibly:** i.e. $P_c(U \rightarrow U') = P_c(U' \rightarrow U)$
  - Accept with Metropolis probability

$$P(U' \leftarrow U) = \min\left(1, \frac{e^{-S(U')}}{e^{-S(U)}}\right)$$

  - If we reject, next config is U again



# Hybrid Monte Carlo

- Big Trick: Update all links at once using Molecular Dynamics
  - Treat each link as ‘canonical coordinate’
  - Assign to each link a ‘canonical momntum’ in the lie algebra su(3)
- Construct a fictitious Hamiltonian

$$H = \frac{1}{2}\sum_{\text{links}} p^2 + S(U)$$

- Simulate Hamiltonian System with partition function:

$$\mathcal{Z} = \int \mathcal{D}U\ \mathcal{D}p\ e^{-H} = \int \mathcal{D}U\ e^{-S} \int \mathcal{D}p\ e^{-\frac{1}{2}\sum_{\text{links}} p^2} = C \int \mathcal{D}U e^{-S(U)}$$

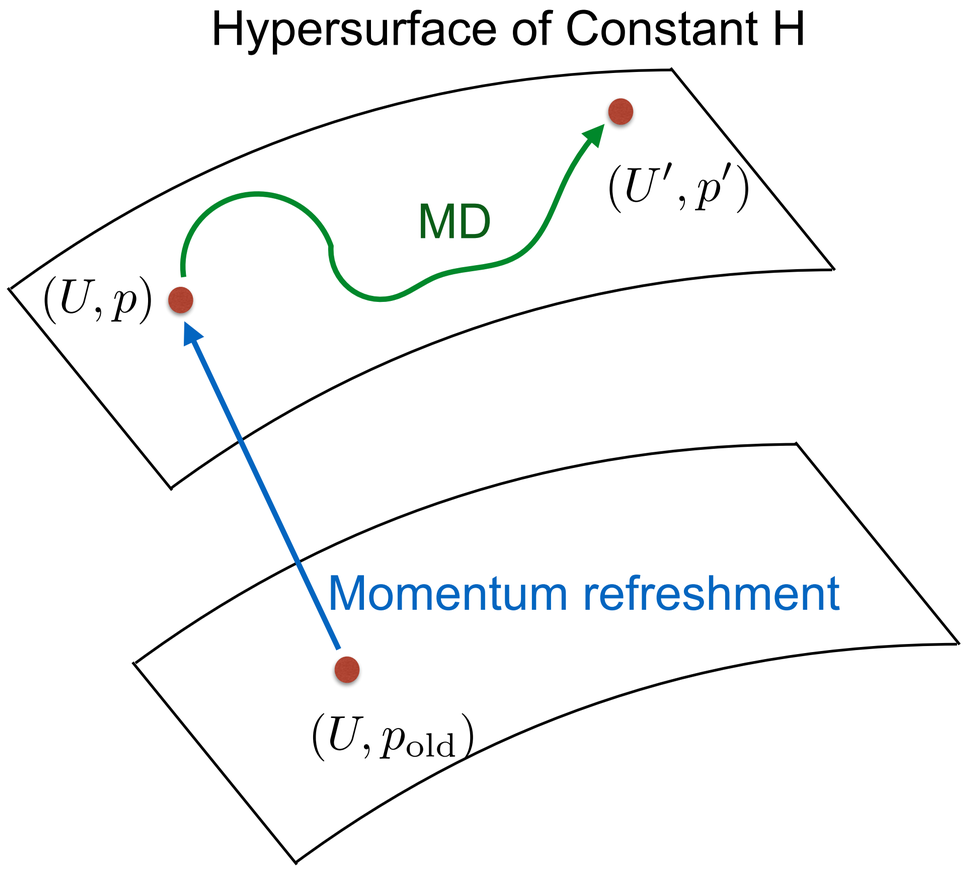
- Momenta have gaussian distribution: easy to generate from heatbath
- Keep the Marginal Distribution of the gauge fields (ignore momenta)

# Hybrid Monte Carlo (HMC)

1. Refresh momenta from Gaussian Heatbath
   - generate (U,p) from (U,$p_{old}$)
2. Compute H = H(U,p)
3. Perform Molecular Dynamics trajectory
   - generate (U',p')
   - MD must be reversible and 'area/measure preserving'
     - To Guarantee Detailed Balance
4. Compute H' = H(U',p')
5. Accept with Metropolis probability

$$P = \min\left(1, e^{-H(U',p')+H(U,p)}\right)$$

6. If (U',p') is rejected, the new state is (U,p)



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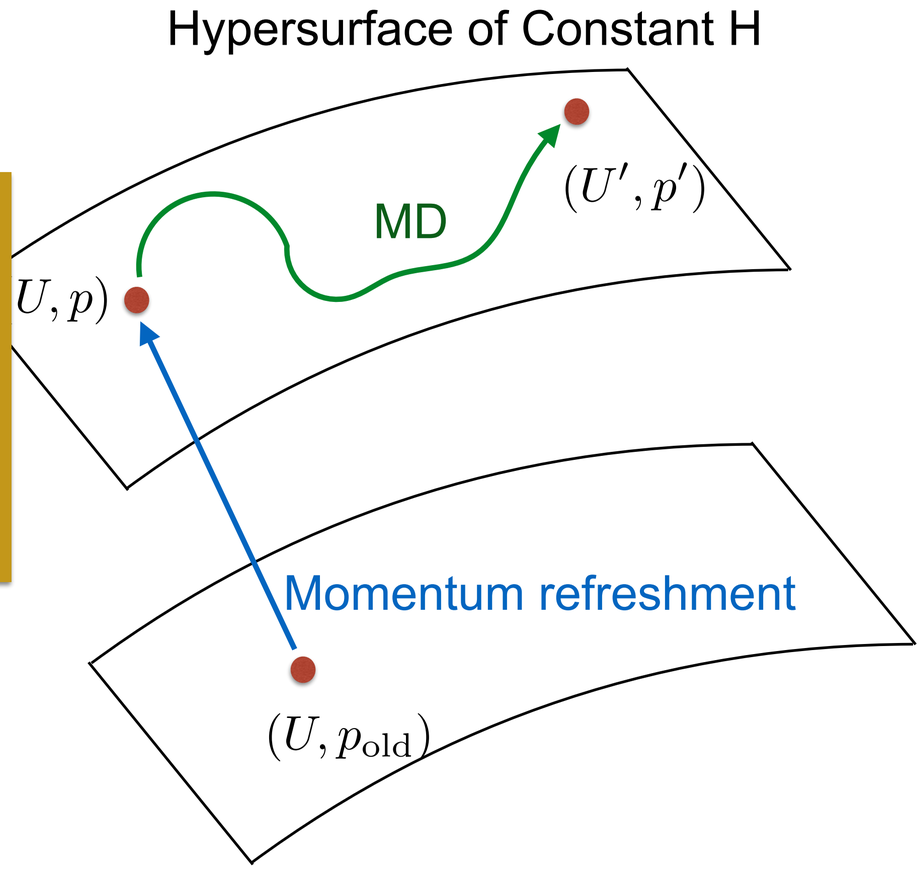
About 95% of time is spent in MD Force Calculations



# MD Forces

- Momentum Update: $e^{\delta\tau \hat{P}} : \; p(\tau + \delta\tau) \rightarrow p(\tau) + \delta\tau F$
- For 2 Flavor Quark Action:

$$F = -\phi^\dagger \left(M^\dagger M\right)^{-1} \left[\dot{M}^\dagger M + M^\dagger \dot{M}\right] \left(M^\dagger M\right)^{-1} \phi$$

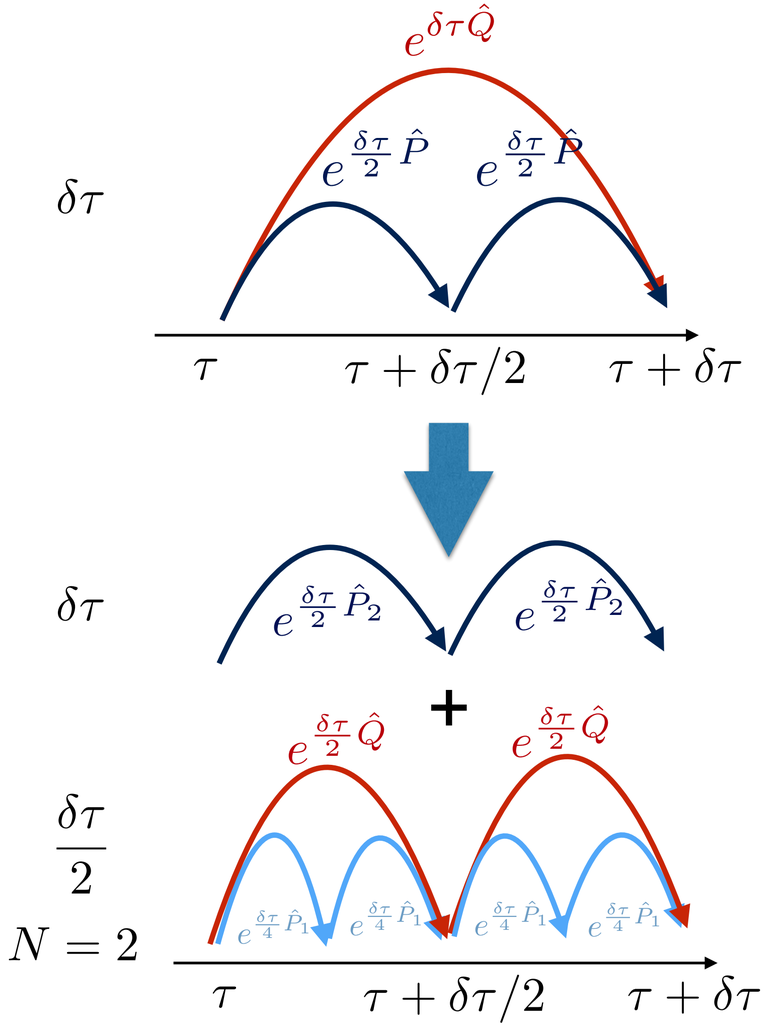
- Need to evaluate:

$$\left(M^\dagger M\right) X = \phi$$

- Here again we need a solver but:
  - System is manifestly Hermitian and Positive definite
  - Common to use two step solve: $M^\dagger Y = \phi$ followed by $M X = Y$ (reduced condition number)
  - M will change as we perform the MD gauge field update, long set-up times for solver may not be as easily amortized as for propagators.

# State Of The Art

- Hybrid Monte Carlo Algorithm
  - Determinant Splitting.
  - **Multiple Time-scale integration using Force-Gradient Term.**
  - Chronological Solution Predictors.
  - **Aggregation Multi-Grid Solver**
- Propagator Calculations
  - **Aggregation Multi-Grid Solver**
- Contractions/Analysis - this varies from calculation to calculation
  - Spectroscopy:  Distillation Method



# Adaptive Multigrid in LQCD

- Critical Slowing down with decreasing quark mass is caused by ‘near zero’ modes of M
- Multi-Grid method based on Adaptive Smoothed Aggregation
  - separate (project) low lying and high lying modes
  - reduce error from high lying modes with “smoother”
  - reduce error from low modes on coarse grid
  - Gauge field is ‘stochastic’, so no geometric smoothess on low modes => algebraic multigrid
  - Setting up restriction/prolongation operators has a cost
  - Easily amortized in Analysis with O(100,000) solves
- ***QCD Version thanks to SciDAC 1,2,3!***
  - Collaboration between R. Falgout & J. Brannick with Boston University Group (R. Brower, K. Clark, R. Babich, C. Rebbi, J. Osborn and others)

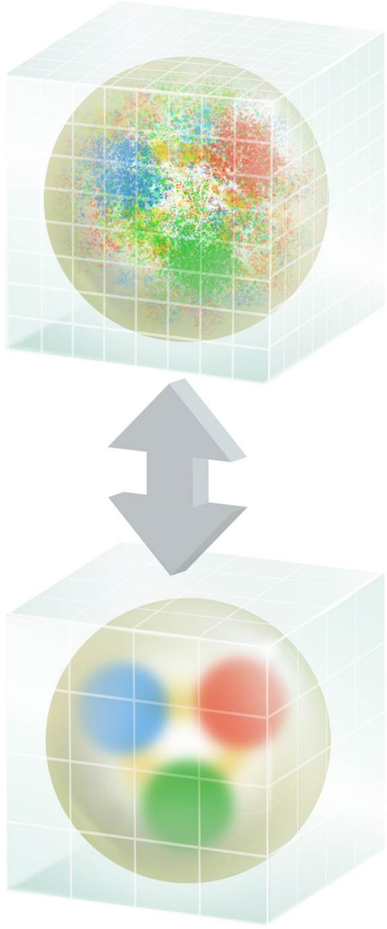
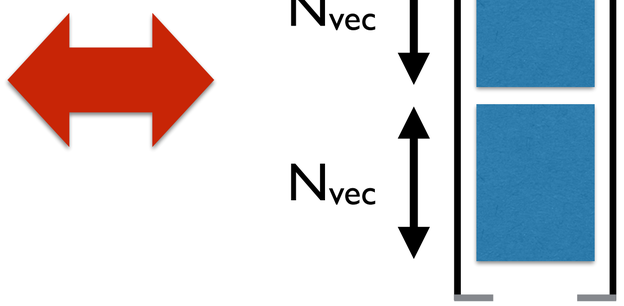


Image Credit: Joanna Griffin, Jefferson Lab Public Affairs

# Block Aggregation

## Restriction via aggregation:

$v_c = R\, v_f$

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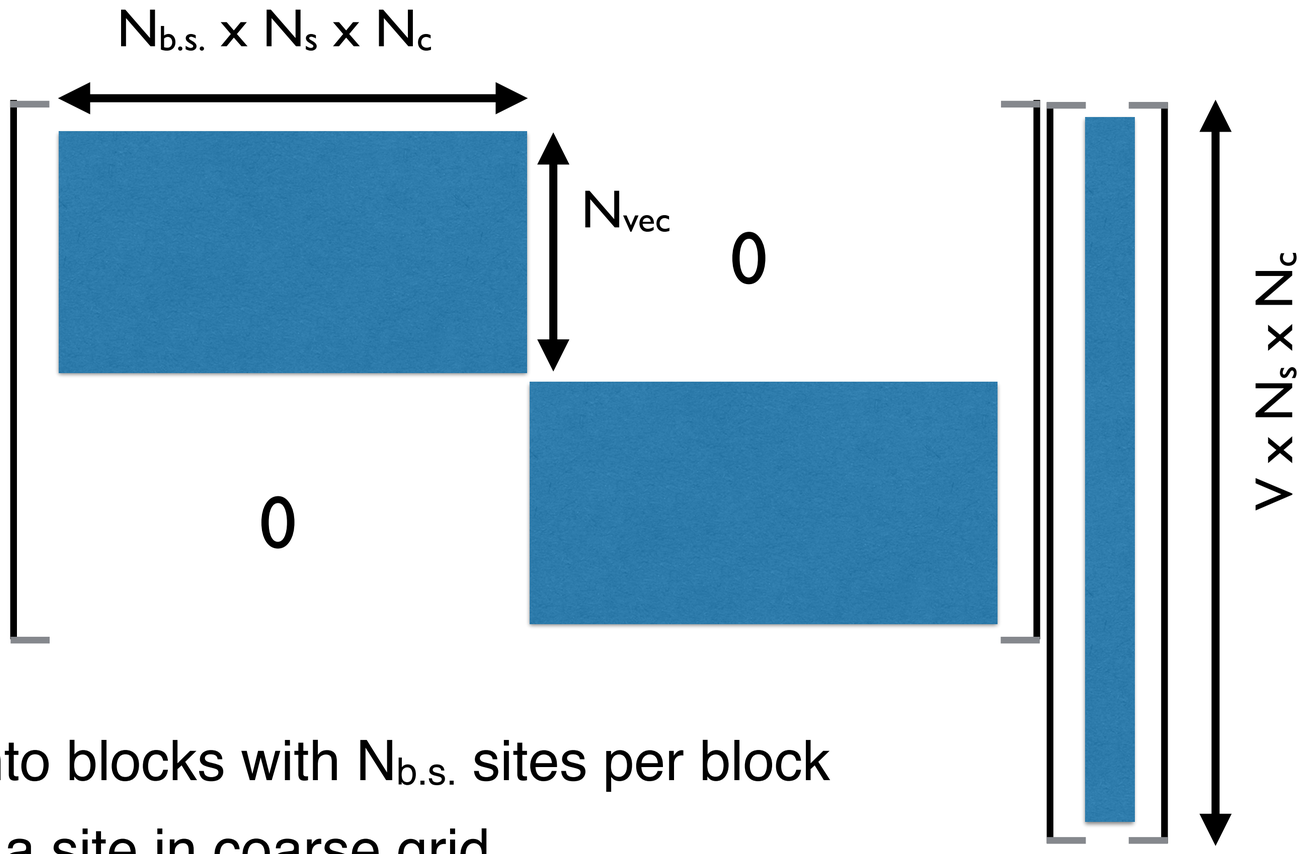
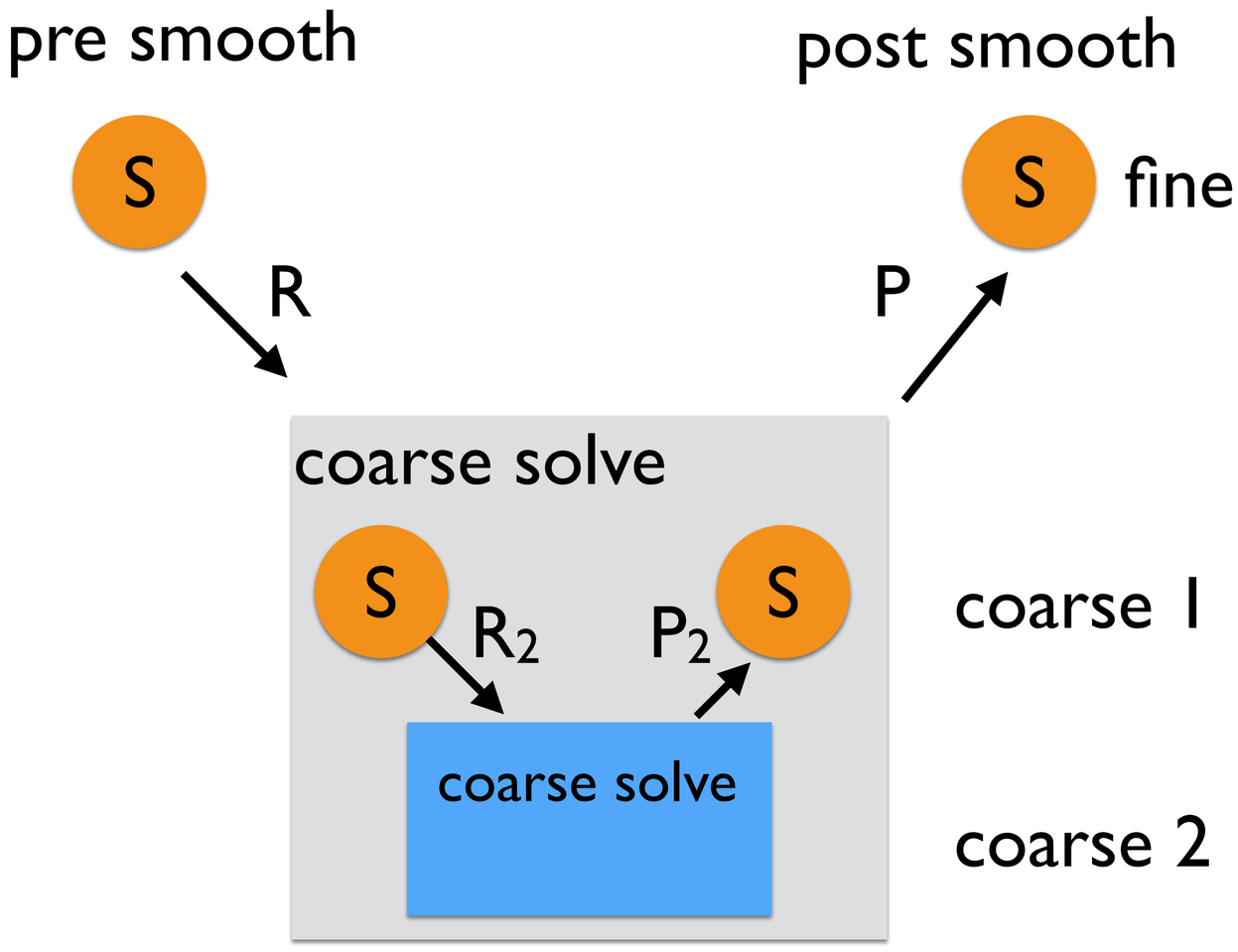



- Generate $N_{vec}$ near-nullspace vectors, 'cut' into blocks with $N_{b.s.}$ sites per block
- Aggregate over blocks: each block becomes a site in coarse grid
- $N_{vec}$ becomes number of 'colors' on each coarse grid site
- Typically use $P = R^{\dagger}$ and Galerkin Coarse Operator $M_c = R\, M\, P$

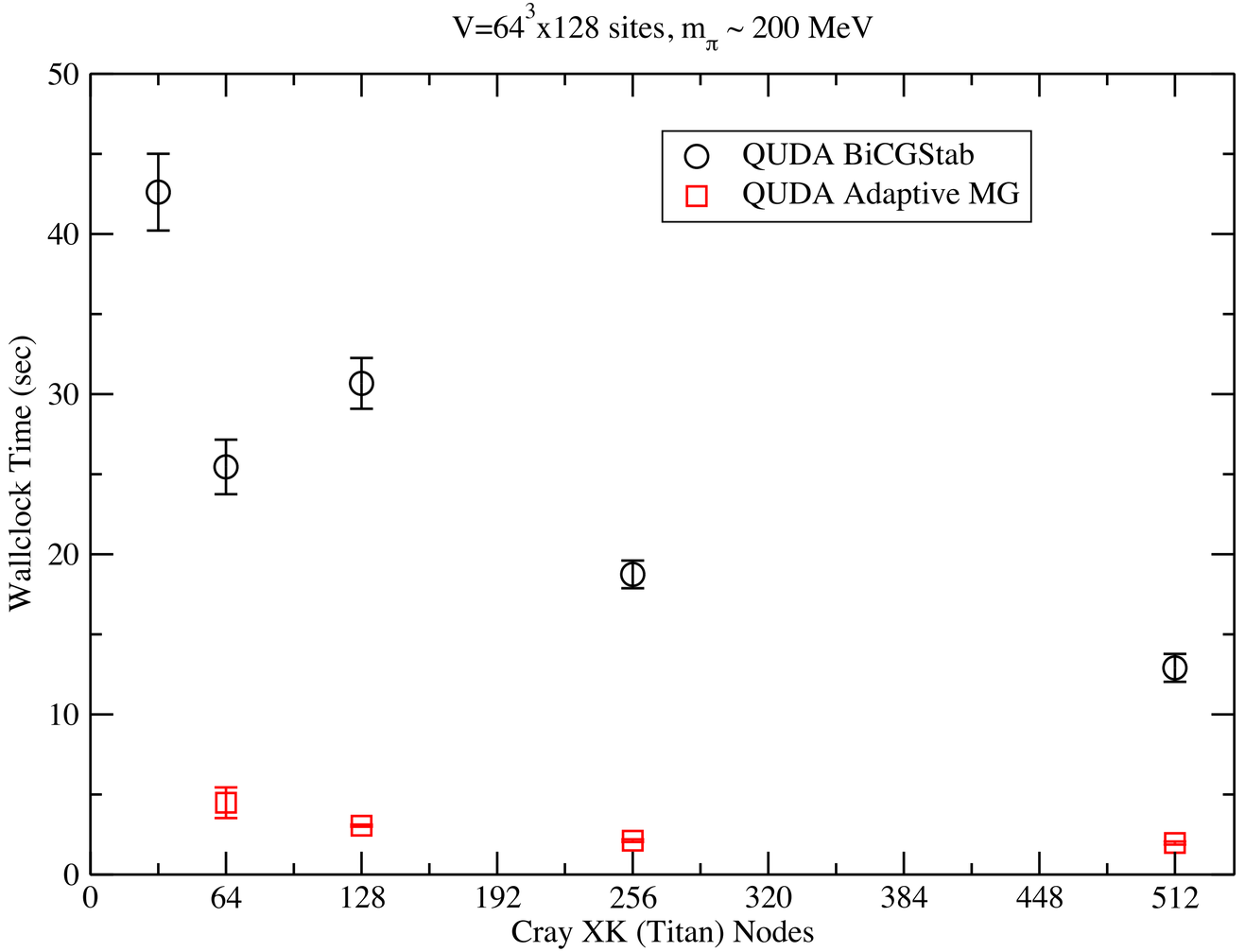
# Typical Implementation

- Outer Flexible Krylov Method
  - e.g. GCR, FGMRES
- MG V-cycle used as a Preconditioner.
  - Null space:
    - Solve M x = 0 for $N_{vec}$ random x, construct R, P
    - more elaborate schemes - research topic
  - Smoother: MR or Block Jacobi
  - 'Bottom Solver':
    - GCR/FGMRES
    - May be deflated (e.g. FGMRES-DR, or explicitly)
    - May be recursively preconditioned (e.g. by MG)
- Very large space of algorithmic combinations/ tuning possibilities: MG cycles, parameters etc.



# Benefits of Multigrid: Speed

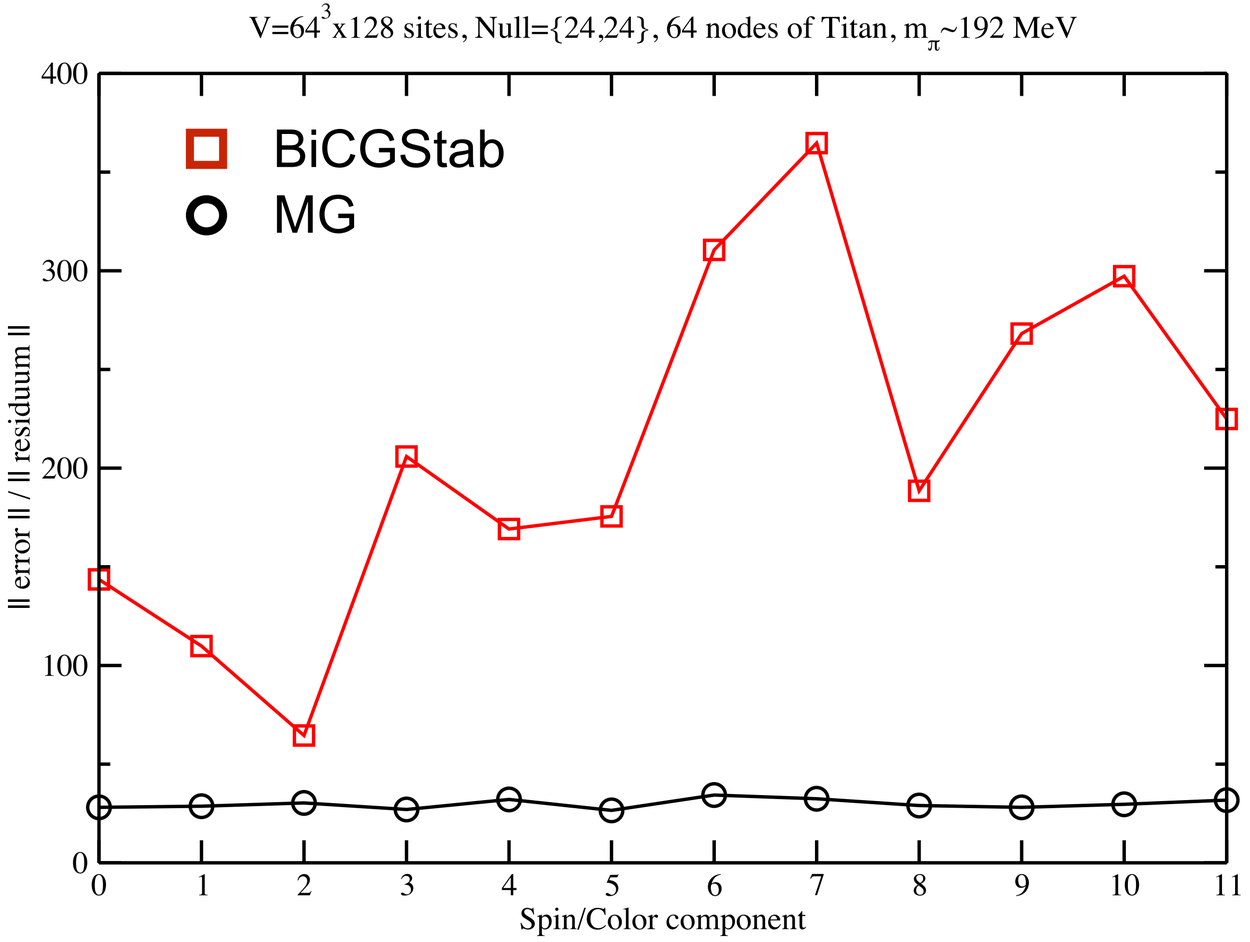
- Coarse Grids capture the troublesome low modes, but with massively reduced number of degrees of freedom.
- Typical Grid Blockings:
  - Level 1: 4x4x4x4 = 256x
  - Level 2: 2x2x2x2 = 16x
  - Overall: 4096x reduction
- MG is a preconditioner
  - reduced precision can be used beneficially without hurting precision of end result
- State of the art GPU implementation in QUDA Library (Clark et. al.)
- Not unreasonable x86 multicore implementation in mg_proto library (Joo)




from K. Clark et. al. SC'16

# Benfits of Multigrid: Optimality

- MG minimizes error, rather than residuum
- Solver is better behaved than BiCGStab
- number of iterations is stable
- ll error ll/ll residuum ll is more stable
- Important for t-to-same-t propagators
  - single precision is good enough BUT:
  - want precision guarantee from solve to solve



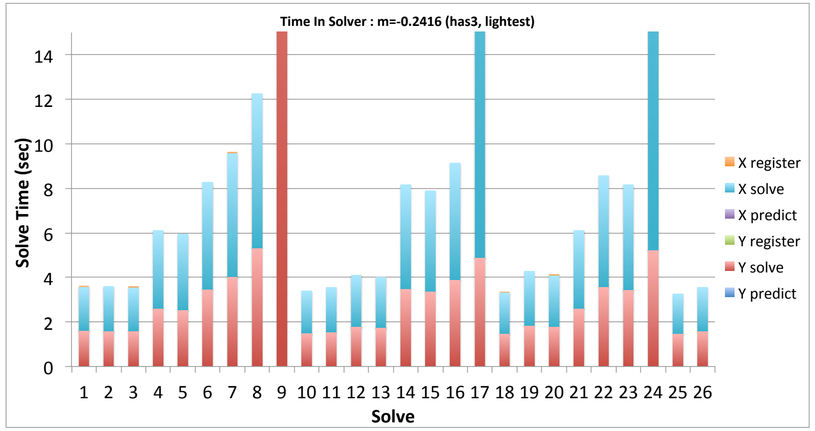

from K. Clark et. al. SC'16 - sneak preview

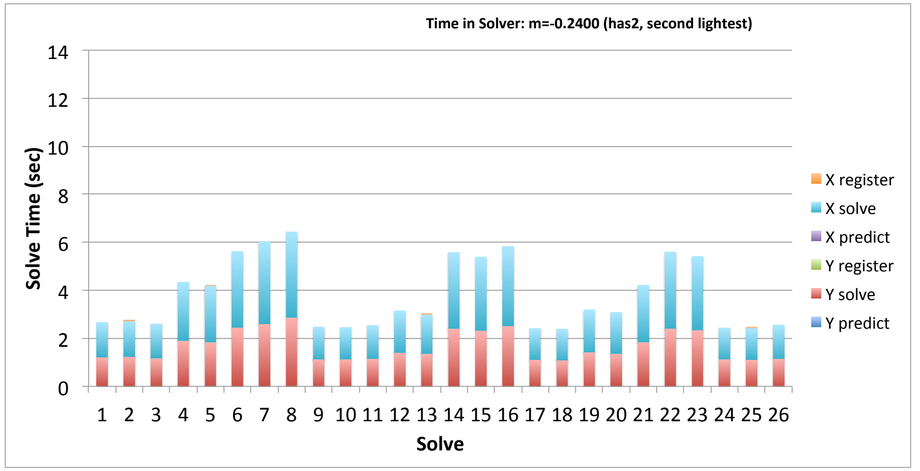
# Multigrid in the HMC

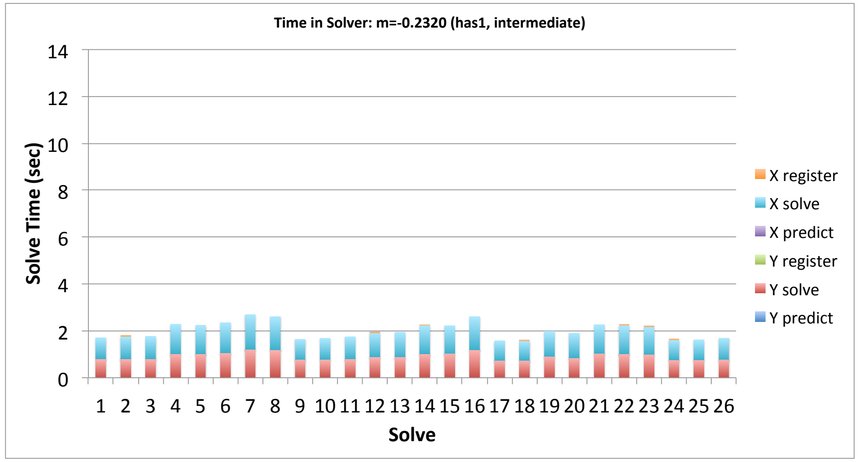
- We focus on the MG implementation in QUDA hooked into Chroma
- Primary Targets: Titan, Summit, Blue Waters and any other big GPU based system we can use
- MG Subspace Management
  - Keep Subspace in Chroma Named Object Store (reuse for solves with several masses)
  - Still need to recompute coarse operators: this must be fast
  - Subspaces lose effectiveness as fields evolve => Refresh when Iteration Threshold reached
  - Keep costs of Subspace Refresh low: use fixed number of iterations (rather than residuum)
  - Two new tunable parameters: Iteration Threshold & Refresh Iterations
- Numerical Experiments: 64^3x128 lattice (a~0.092fm, mpi ~ 172 MeV)
  - Production Isotropic Lattice

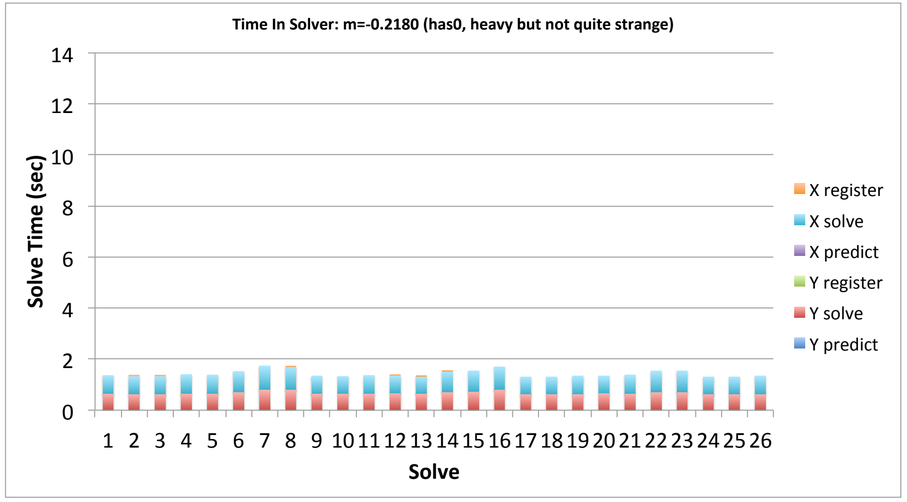
# Multigrid Behavior

- Only the lightest mass really matters — as expected. And as shown before by M. Lin the preconditioner doesn't degrade much for heavier masses

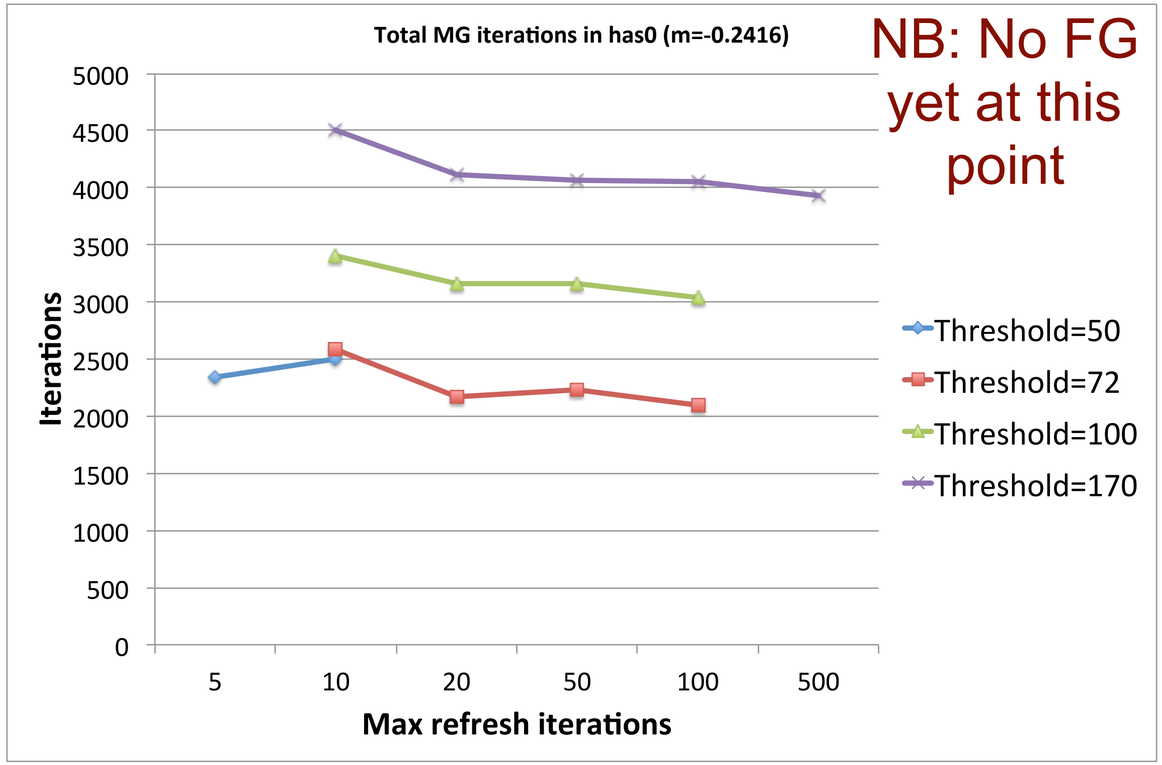


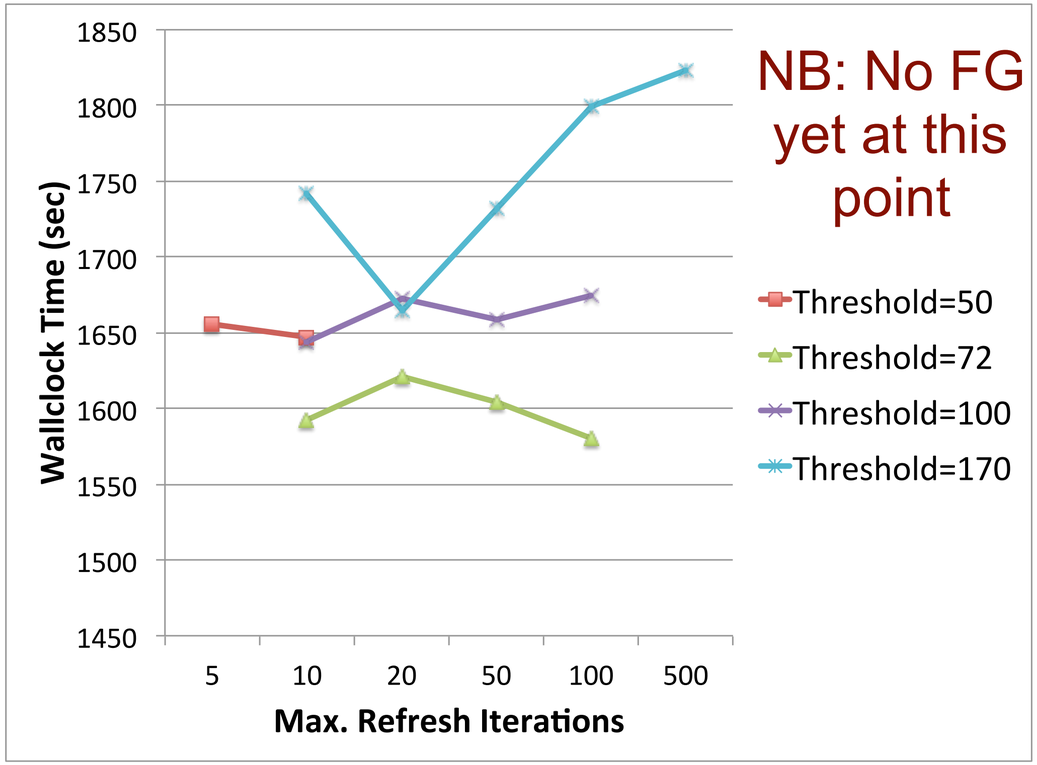



# Multigrid Tuning

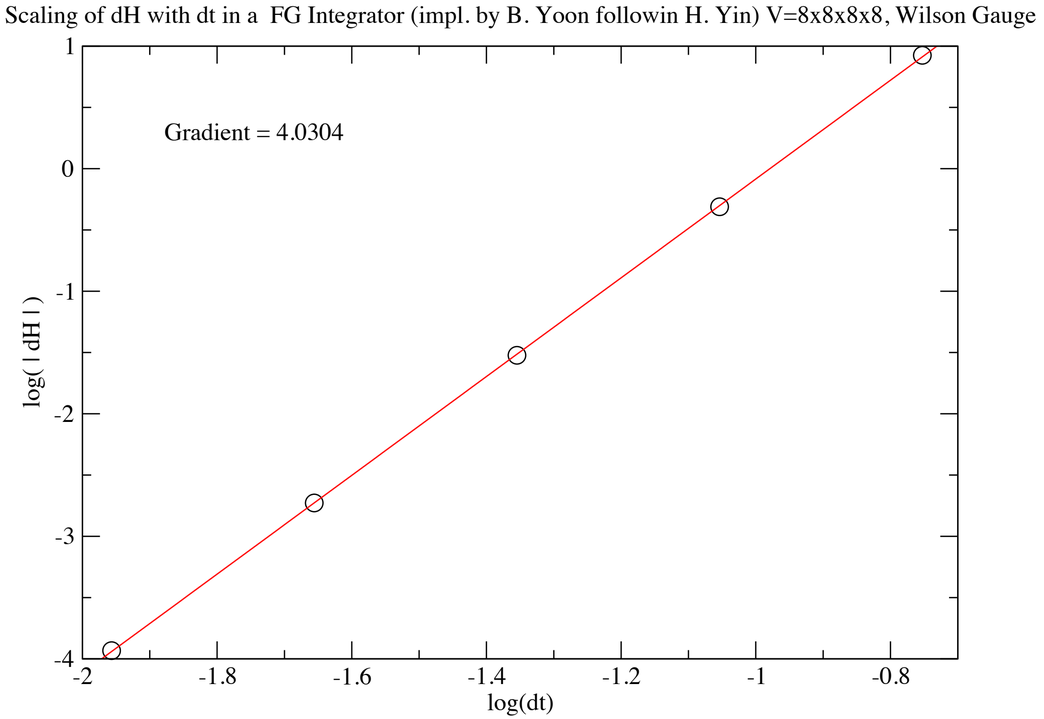


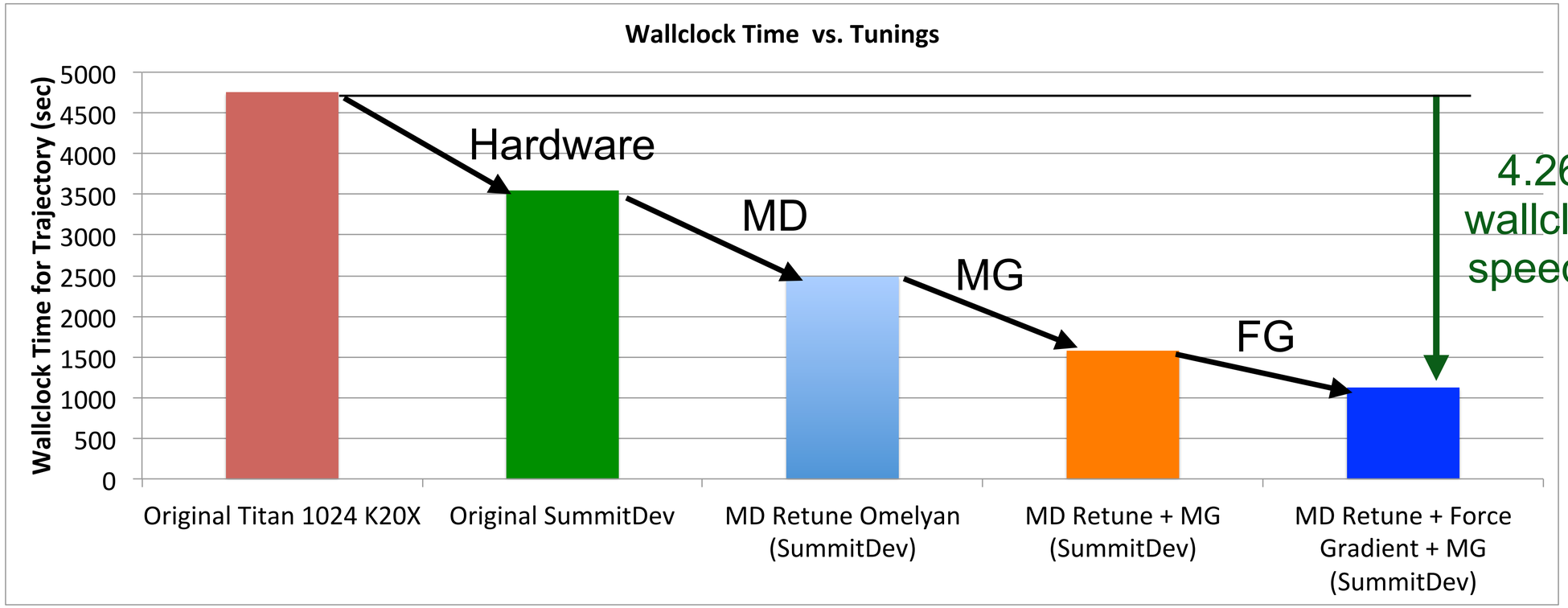

- Outer MG iterations insensitive to refresh iterations once refresh iters > 20 or so
- In terms of time, it is not immediately clear where the point is…
  - For Threshold=170 it is what I expect: there is a nice minimum (fewer iters=>worse space, more iters=> expensive)
  - For Threshold=72, we refresh sufficiently often to keep a low iteration count?

# Force Gradient Integrator

- Standard 4th order integrator following Omelyan requires 5 force evaluations per step (4MN5FV version)
- Omelyan 2nd order intergrator requires 3 force evaluations per step
- Force gradient integrator (Clark, Kennedy, Silva) following H. Yin and Mawhinney's exponential trick needs 3 force evaluations + 1 auxiliary force gradient evaluation, but is 4th order
  - Saves on solves compared to 4MN5FV
  - 4th order so volume scaling of cost is $V^{9/8}$.



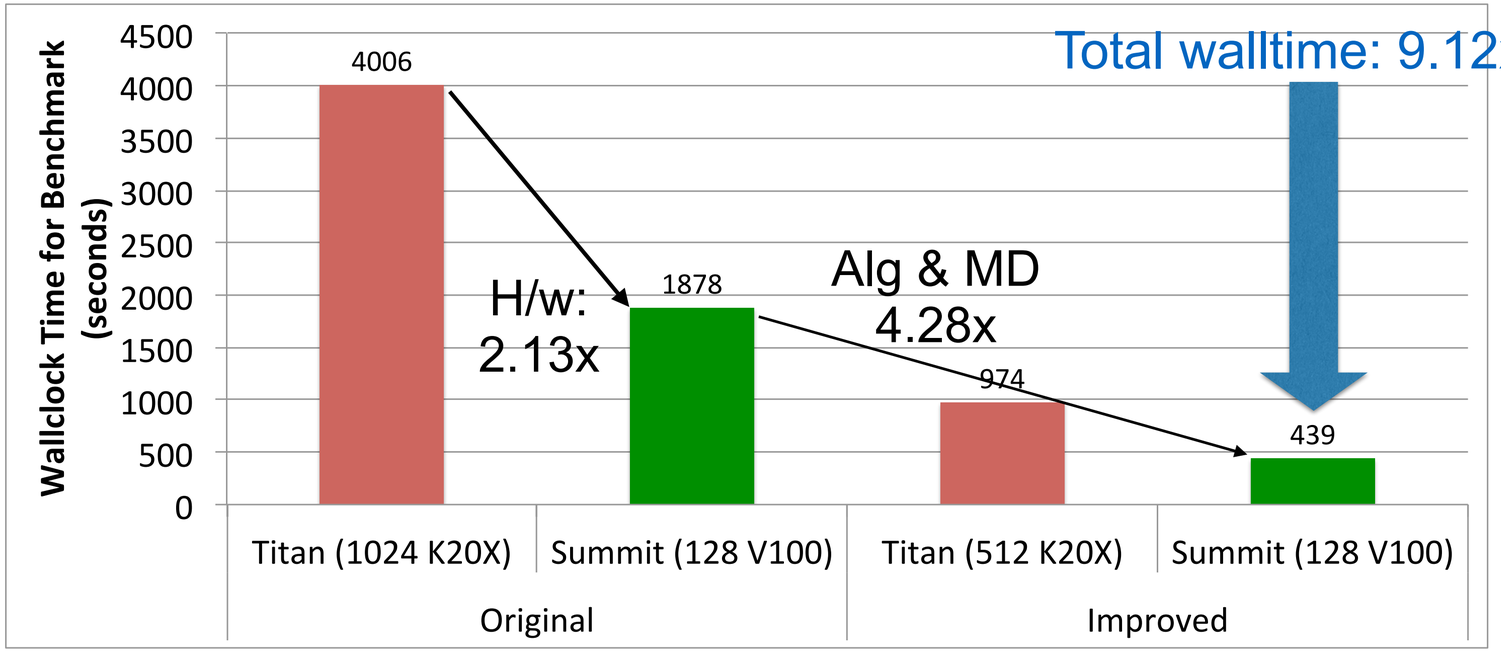
# Summit Dev Gains.




- 4.25x wallclock speedup on SummitDev
- On Titan, after all algorithmic optimizations on 512 nodes: ~974 sec per traj

# Summit Gains

*SciDAC Highlight In 2018!*




*Can We Get To 100x ?*

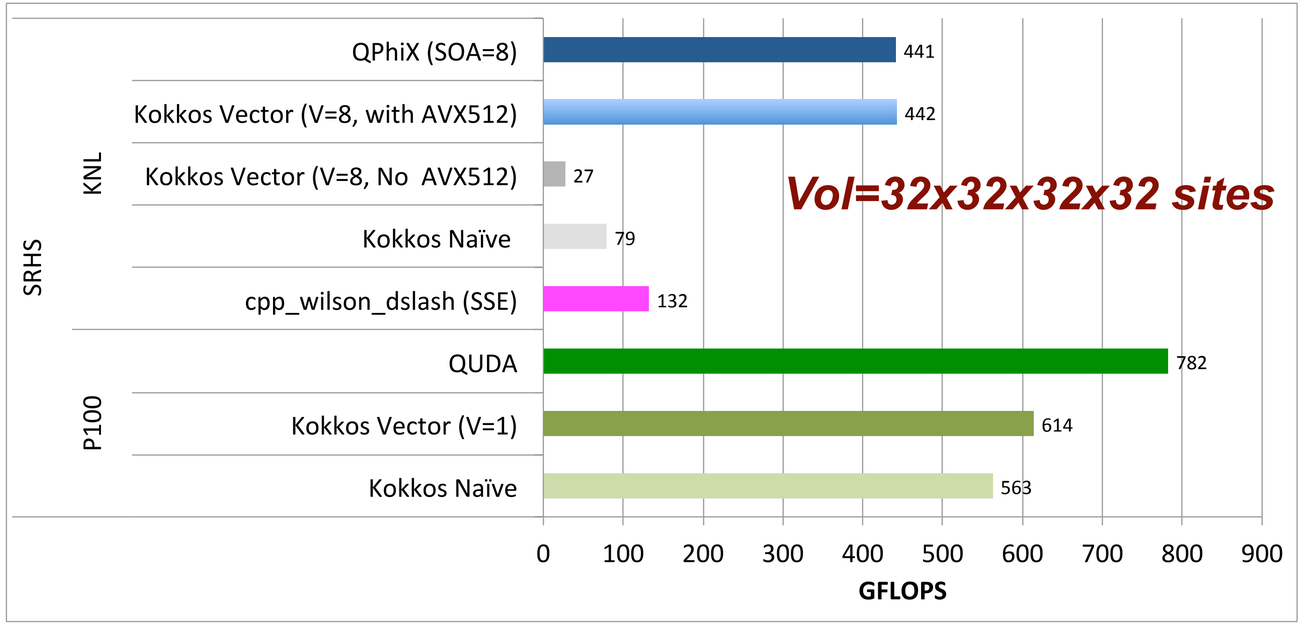
- Combined Hardware x Algorithm & MD Retuning Walltime gain: **9.12x**
- 8x reduction in GPUs: Integrated gain: **73x**. (Contribution to 2018 ECP FOM)
- Updated: more QUDA optimizations (reduced prec chrono vecs etc.): 392.6 sec
  - **10.2x walltime x 8-fold GPU reduction => 81.6x (Contribution to 2019 ECP FOM)**

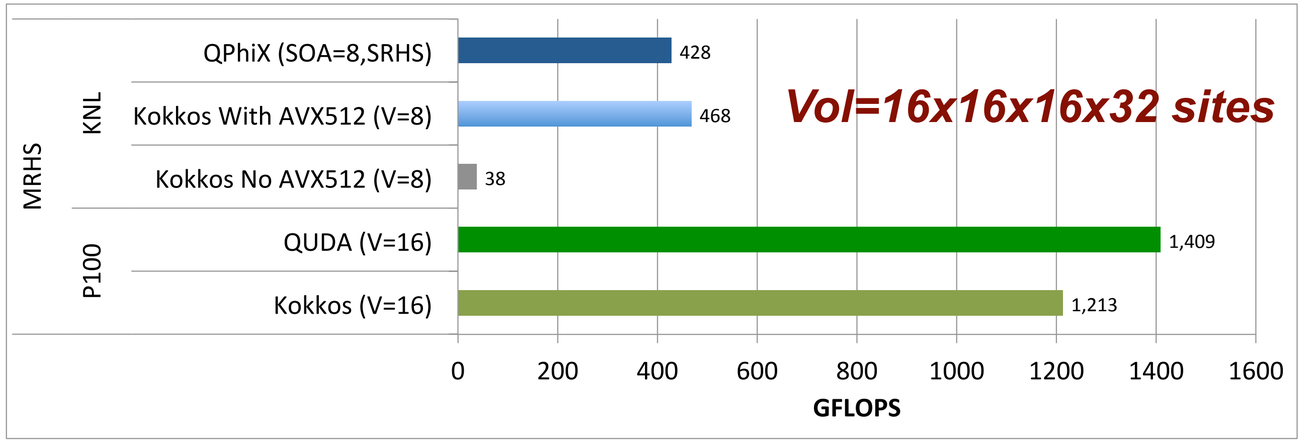
# Future Work/Challenges

- Raw Performance through Multi-RHS solvers
  - N-RHS at a time can in principle reap N-fold reuse of gauge field (*subject to other bottlenecks)
  - Interesting MRHS algorithms out there (e.g. using auxiliary RHS, or for changing matrices)
- Scaling Challenges
  - Usual MG scaling challenges (data parallel degrees of freedom get coarsened away)
  - Use domain decomposed preconditioners (?)
  - Multi-RHS can help with strong scaling in MG (more network friendly)
  - Multi-shift solvers for rational approximations in RHMC are still a challenge
- Better MD Integrators?
- More efficient Markov-Chain Monte Carlo methods ?  (also studied in LQCD ECP)
- Performance Portability (we are OK currently, but Aurora/Frontier will be v. new)

# Current Kokkos Performance Summary

- SRHS Case:
  - ***Kokkos Vectorized Dslash with AVX512 and tuned blocking matches QPhiX on Cori KNL node (68 cores, 272 threads)***
  - Unvectorized & No AVX cases are slow
  - Kokkos Naive CUDA version is 72% of QUDA on P100 (SummitDev)
  - ***Vectorized (but V=1) QUDA version benefits from block tuning, memory & locality optimizations and md_parallel_for: 79% of QUDA on P100 (SummitDev)***
- MRHS Case:
  - ***Kokkos With AVX512 exceeds corresp. QPhiX SRHS performance on Cori KNL node for 8 RHS***
  - Kokkos Without AVX512 is very slow
  - ***Kokkos CUDA version is 86% of QUDA for 16 RHS on SummitDev (P100)***



# Summary

- A variety of applied maths topics touched in LQCD
- Linear Solvers have traditionally received most focus
- Adaptive Multi-grid for Wilson Clover Fermions (developed thanks to SciDAC) has been a game changer for LQCD - other fermion actions in development
- Looking to the future we always need better solvers, better MD integrators and better Monte-Carlo methods
- A large focus with machines coming down the road is performance portability
  - Encouraging early Kokkos experiences. Would like to start looking at Kokkos SIMD types, and potentially performance portable Batched BLAS (Kokkos Kernels?) Also looking at SyCL and OpenMP-5 for future architectures (ECP).
- Our SciDAC project also has components looking at Optimization and Workflow.
- Questions?

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